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Modeling observed saturation overshoot with continuum additions to standard unsaturated theory

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Abstract

In uniform soils that are susceptible to unstable preferential flow, the water saturation exhibits a nonmonotonic profile upon continuous infiltration. This overshoot cannot be described by the conventional Richards equation. Here, solutions to the infiltrations using a popular nonequilibrium extension to the Richards equation are obtained using the traveling wave nature of the saturation profile. Quantitative comparisons are made to recent measurements of saturation overshoot. The nonequilibrium solutions can be made to fit the flux range of the overshoot, but the fit to the tip saturations is fair to poor at best. Also, small changes in porous media size and roughness require large changes in the magnitude of the nonequilibrium term to match the flux range. The results suggest that the nonequilibrium capillary pressure does not include the correct physics that controls the overshoot.
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1. Introduction

It has been shown that constant flux infiltrations into sandy porous media can produce a water saturation and water pressure profile in which the saturation (and pressure) overshoots at the initial wetting front before settling down to its asymptotic value [23,9,3]. This saturation overshoot at the wetting front has been hypothesized to be the cause of gravity driven fingering [9,6,5]. As pointed out by Jean-Yves Parlange [16], the parameters that control fingering are the saturation and pressure behind the wetting front, as these are necessary inputs to most if not all models which predict infiltration stability and finger widths [2,18,10,25].

Recently, it has been shown that overshoot simply cannot be described by the Richards equation [6,5], the primary unsaturated flow equation. The Richards equation, which gives the time change of water content in a porous medium, is simply a combination of conservation of mass, the Darcy–Buckingham unsaturated flux equation, and the soil characteristic pressure–saturation curve [14,4]. Implicit in the Richards equation is the fact that one can define a length scale where properties such as porosity, conductivity, and saturation can be considered continuous [1]. Although widely successful for modeling almost all observed water flows, it has been argued that additional continuum terms are necessary, in particular for when the local saturation changes quickly [11,7,12].

The observed overshoot would seem to give credence to the necessity of adding additional continuum terms to the Richards equation to reproduce the observed phenomena [7,8]. Eliassi and Glass [7] considered three possible additional terms and from numerical simulations using one of them [8] produced saturation patterns which qualitatively matched up with those seen in gravity driven fingers.

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Clearly quantitative comparisons are needed between the possible continuum additions and measurements of saturation overshoot. Recently, saturation overshoot has been measured in detail as a function of grain size, grain angularity, applied flux, and initial water saturation [3]. These detailed measurements provide a benchmark for studying additional terms of continuum models, and their efficacy for reproducing saturation overshoot.

In this paper, we use the traveling wave property of the infiltrating water content in space to convert the Richards equation plus any additional continuum terms to an ordinary differential equation. Solutions of this ODE are found for the additional nonequilibrium capillary pressure term [13,12] which has been one of the most popular additions to continuum theory. These solutions are then fir to the previously measured overshoot [3]. The infiltrating flux range over which overshoot occurs can be matched with this additional term, but the fit to the tip saturations is poor and the magnitude of the term must be varied greatly from sand to sand.

2. Theory and model

Saturation overshoot is modeled in a 1-D space with the only direction being z the vertical direction. Assuming the only forces acting on the water are gravitational and capillary, with z positive downward the Darcy–Buckingham flux is

$$q = -K(\theta)\frac{\partial h_w}{\partial z}, \tag{1}$$

where $K(\theta)$ is the unsaturated conductivity which depends on the volumetric water saturation θ and

$$h_w = P_w - z \tag{2}$$

is the total head in units of cm of water, and consists of the pressure term (P_w) and the gravitational term. From this and conservation of mass, the Richards equation is obtained [14],

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\left(\frac{\partial P_w}{\partial z} - 1\right)\right]. \tag{3}$$

Let this be our starting point. It is useful to define the diffusivity as

$$D(\theta) = K(\theta)\left(\frac{\partial P_w}{\partial \theta}\right). \tag{4}$$

Note this assumes a one to one dependence of the capillary pressure of the water on the saturation. This is known to have hysteresis on imbibition and drainage, and an additional nonequilibrium component will be added shortly.

Thus the Richards equation can be written only in terms of θ,

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[D(\theta)\left(\frac{\partial \theta}{\partial z}\right)\right] - \frac{\partial}{\partial z}K(\theta). \tag{5}$$

Infiltration experiments have shown that the saturation profile can be described as a traveling wave [21], once far enough away from the soil surface. Thus $\theta(z,t)$ can be written as $\theta(z - vt)$ which will give a solution propagating downward at a velocity of v. Following Philip [19] and Parlange [17], a new variable $\eta = -(z - vt)$ can be introduced, the partial differentials become simple derivatives, and the PDE collapses to an ODE

$$v\frac{d\theta}{d\eta} = \frac{d}{d\eta}\left[D(\theta)\left(\frac{d\theta}{d\eta}\right)\right] + \frac{d}{d\eta}K(\theta). \tag{6}$$

Using the boundary conditions of

$$z = +\infty, \quad \eta = -\infty; \quad \theta = \theta_0, \quad \frac{d\theta}{d\eta} = 0, \tag{7}$$

at the bottom of the column, and

$$z = -\infty, \quad \eta = +\infty; \quad \theta = \theta_1, \quad \frac{d\theta}{d\eta} = 0, \tag{8}$$

at the top of the column, gives the solution of

$$v(\theta - \theta_0) = D(\theta)\frac{d\theta}{d\eta} + (K(\theta) - K(\theta_0)), \tag{9}$$

with the wave velocity given by

$$v = \frac{K(\theta_1) - K(\theta_0)}{(\theta_1 - \theta_0)}. \tag{10}$$

Eq. (9) can be solved by a simple integration. This solution is known not to give overshoot as long as the unsaturated conductivity is positive and increasing faster than linearly with saturation, and that the diffusivity is positive. Hysteresis does not play a role as the saturation is always increasing (no overshoot) and the soil remains on the wetting curve.

This same traveling wave solution is easily adaptable to include a dynamic nonequilibrium capillary term as suggested by Hassanizadeh and Gray [13,12,5]. They postulate that the dynamic (actual) pressure is related to the static capillary pressure through

$$P_w = P_w(\theta) + \tau(\theta)\frac{\partial \theta}{\partial t}, \tag{11}$$

where $P_w(\theta)$ is the static capillary pressure–saturation curve (either imbibition, drainage, or scanning, in this case it will be imbibition). The coefficient $\tau(\theta)$ gives the magnitude of the dynamic effects, and it has the SI units of kg/ms. It is typically chosen to be a constant with saturation, but it has been suggested that it may also vary with saturation [12], so the dependence is kept explicit for now. Of course, $\tau = 0$ returns the static capillary pressure, and conventional Richards equation.

Substituting this pressure term into Eq. (3) gives

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial z}\left[D(\theta)\left(\frac{\partial\theta}{\partial z}\right)\right]-\frac{\partial}{\partial z}K(\theta)+\frac{\partial}{\partial z}\left[K(\theta)\frac{\partial}{\partial z}\left(\tau(\theta)\frac{\partial\theta}{\partial t}\right)\right], \tag{12}$$

where the diffusivity is from the static curves. Using the same traveling wave solution results in

$$v\frac{d\theta}{d\eta}=\frac{d}{d\eta}\left[D(\theta)\left(\frac{d\theta}{d\eta}\right)\right]+\frac{d}{d\eta}K(\theta)+v\frac{d}{d\eta}\left[K(\theta)\frac{d}{d\eta}\left(\tau(\theta)\frac{d\theta}{d\eta}\right)\right]. \tag{13}$$

Again integrating with the same boundary conditions, and rearranging gives a 2nd order ODE for the saturation in terms of η,

$$vK(\theta)\frac{d}{d\eta}\left(\tau(\theta)\frac{d\theta}{d\eta}\right)+D(\theta)\frac{d\theta}{d\eta}+K(\theta)-K(\theta_0)-v(\theta-\theta_0)=0, \tag{14}$$

with the velocity given as before (Eq. (10)). This can be solved numerically by integrating θ from the bottom boundary condition. As will be seen this equation can produce overshoot for certain values of τ and v.

Eliassi and Glass [7] propose other possible extensions which can be added to right hand side of the Richards equation, that they call a hypodiffusive and hyperdiffusive terms respectively,

$$R_{\text{hypo}}=\frac{\partial}{\partial z}\left[F(\theta)\frac{\partial}{\partial z}\theta\right], \tag{15}$$

$$R_{\text{hyper}}=-\frac{\partial}{\partial t}\left[T(\theta)\frac{\partial}{\partial t}\theta\right], \tag{16}$$

where $F(\theta)$ and $T(\theta)$ are postulated to be unknown functions of saturation. These can be incorporated using the same traveling wave solution and in either case, one arrives at a first order ODE exactly as given by Eq. (9), with a new effective diffusivity D^* given by

$$D^*_{\text{hypo}}(\theta)=D(\theta)+F(\theta), \tag{17}$$

$$D^*_{\text{hyper}}(\theta)=D(\theta)-v^2T(\theta), \tag{18}$$

for the hypodiffusive and for the hyperdiffusive term respectively. In these cases overshoot is created when there is a saturation region where the effective diffusivity is negative (through a negative $F(\theta)$ or a positive $T(\theta)$). This forces the saturation to have a discontinuity over this saturation region, as seen in the numerical solutions of Eliassi and Glass [8]. The exact taking off and landing points of the discontinuity have yet to be determined, but in either case it cannot be solved by a continuous integration as can be for the nonequilibrium term. Therefore the solution to the 2nd order ODE with the nonequilibrium capillary pressure is focused on.

Table 1
Physical parameters for the three sands used in the experimental study [3]

Sand	d_{50} (mm)	Shape	K (cm/min)	ϕ	α (cm^{-1})	n
12/20	1.105	Spherical	30	0.35	0.303	4.98
20/30	0.713	Spherical	15	0.35	0.177	6.23
Grey	0.96	Angular	32	0.40	0.330	4.14

The soil characteristic parameters where taken on imbibition. For each sand the residual water content was assumed to be $S_r = 0$ (appropriate for imbibition), and in the Mualem unsaturated conductivity parameter (l) was taken as 1.

The integration is performed using the ODE solvers in MATLAB (Mathworks). The soil characteristic curves used were from the same three sands from which the overshoot was measured [3]. The van Genuchten [24] formulation for the soil characteristic curves was used, and the parameters for the sands are listed in Table 1.

The coefficient of the dynamic term τ was chosen to be independent of saturation (constant τ), and was adjusted so the solution to Eq. (14) provides the best looking fits to the previously measured overshoot [3]. In particular, attention was placed on making the flux range for which saturation overshoot appears from Eq. (14) match that seen in recent experiments. Solutions were obtained using nonhysteretic and hysteretic soil characteristic curves. Either set of characteristic curves produced the same magnitude of saturation overshoot, as the magnitude of the overshoot is determined entirely on the imbibition branch of the soil characteristic curve. Saturation dependent τ of varying functional forms were also attempted to fit the data, and are discussed in the results.

3. Results

Fig. 1 shows self similar infiltration solutions to Richards equation with the additional nonequilibrium term. For this solution, 20/30 sand parameters were used for the soil characteristic curves, the τ parameter was chosen to be a constant of 4×10^5 kg/ms and the initial water content was set to 0.002 [27]. The additional term clearly does produce large overshoot at moderate fluxes, and minimal or no overshoot at very low fluxes. This is similar to that seen in previous experiments for fingering [26] and one-dimensional displacements [3]. A larger τ produces a greater flux range over which overshoot occurs, and a smaller τ produces a smaller flux range of overshoot. The parameter τ can then be adjusted to achieve the same range of fluxes over which overshoot takes place in the experiments.

Fig. 2 shows the tip and tail saturations previously measured for the initially dry 20/30 sand [3], with the best fit using a constant τ (solid line). The solutions using a constant τ match the overshoot range well, but

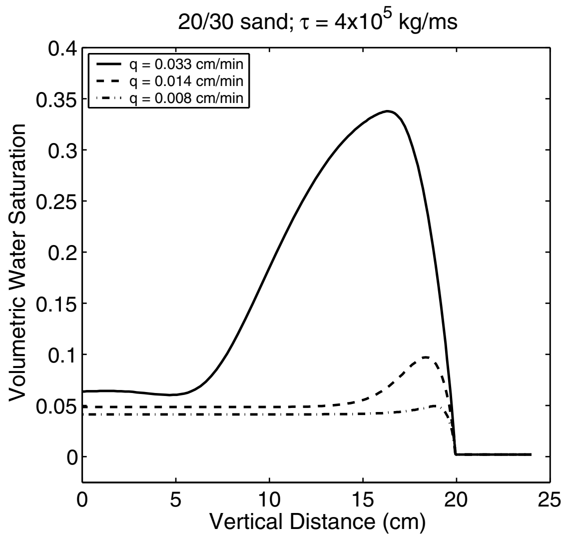

Fig. 1. Calculated traveling wave saturation profiles for imbibition using the Richards equation plus the nonequilibrium pressure. At low infiltrating fluxes, little or no overshoot is seen, but at moderate and higher fluxes, the saturation exhibits overshoot.

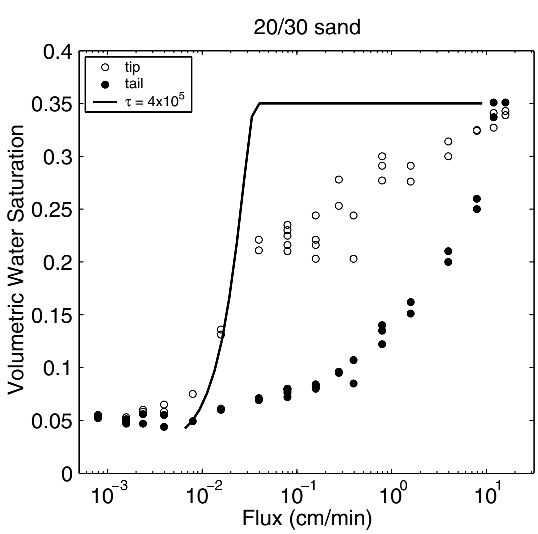

Fig. 2. Calculated tip saturations (solid line) versus flux using $\tau = 4 \times 10^5$ kg/ms compared to experimental measurements of the tip and tail saturations for dry 20/30 sand [3]. The value of τ was chosen to match the flux range of the observed overshoot.

the tip saturation match is fair, with the saturation in the tip going quickly to fully saturated, once overshoot occurs. In contrast, the experimental data shows logarithmically increasing tip saturation with increasing flux.

Fig. 3 shows the tip and tail saturations previously measured for the initially dry 12/20 sand [3], with the best fit for a constant τ (solid line). The overshoot range can again be fit well, but the tip saturation using a constant τ is poor, even with the large scatter in the experimental data. In addition, the magnitude of τ needed to achieve these fits is a factor of 10 greater than that seen

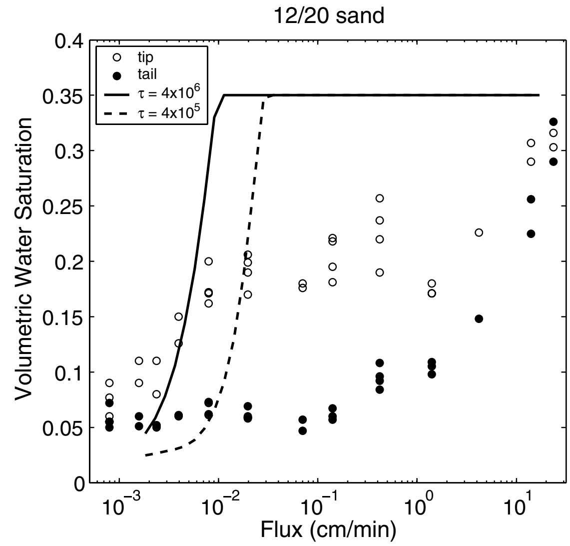

Fig. 3. Calculated tip saturations (solid line) versus flux using the best fit $\tau = 4 \times 10^6$ kg/ms compared to experimental measurements of the tip and tail saturations for dry 12/20 sand [3]. The fit is poorer than that seen for the 20/30 sand and the best τ is an order of magnitude greater than that for the 20/30 sand (shown in dashed line).

in the 20/30 sand. The dashed line shows the tip saturations using the τ obtained from the 20/30 sand and the 12/20 soil characteristics. Clearly the same τ does not seem to work well from sand to sand, even with the only change in sand being the grain size. Note that the τ from the 20/30 sand produces roughly the same range and magnitude of overshoot as seen in the 20/30 sand (see Fig. 2) despite the difference in soil parameters from 20/30 to 12/20 sand.

Fig. 4 shows the tip and tail saturations previously measured for the initially dry grey sand [3], with the best fit for a constant τ (solid line). Here the fit is quite poor even with lowering τ by an order of magnitude from the 20/30 sand and two orders of magnitude from the 12/20 sand. Again, the τ obtained from the 20/30 sand (dashed line) does not work for this slightly larger more angular sand.

In addition to a constant τ, different saturation dependent τ's were also attempted to fit the observed overshoot. Three different functional forms were attempted: (a) a τ that increases with water content $\tau = \tau_0 S^\beta$ (where $S = \theta/\phi$ is the saturation); (b) a τ that decreases with water content $\tau = \tau_0(1 - S)^\beta$, and a τ that is large near saturation and low water content and is smallest in the mid-range with $\tau = \tau_0|0.5 - S|^\beta$. In each case the parameters τ_0 and β were adjusted to produce the best fit to the overshoot range. Fig. 5 shows the results of these fits. It was found that the exponent β did not change the quality of the fits drastically, so β was held constant at 1 for simplicity and to limit the fitting parameters. Clearly, cases (b) and (c) provided fits that were roughly equal to the constant τ case, and thus pro-

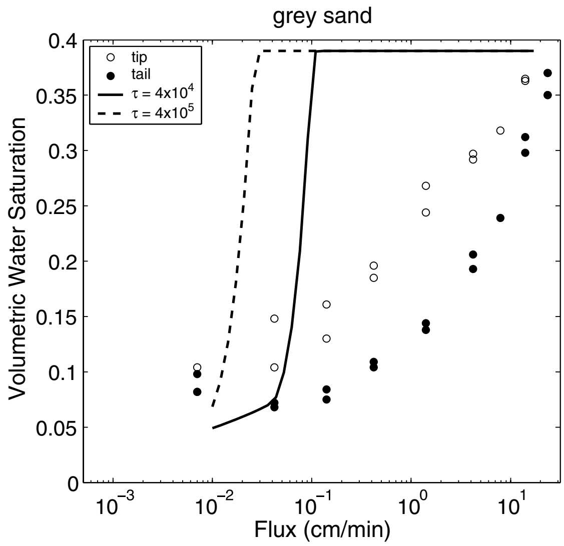

Fig. 4. Calculated tip saturations (solid line) versus flux using the best fit $\tau = 4 \times 10^4$ kg/ms compared to experimental measurements of the tip and tail saturations for dry 12/20 sand [3]. Even the best fit is poor, and the best τ is an order of magnitude less than that for the 20/30 sand (shown in dashed line), and two orders of magnitude less than that from the similarly sized 12/20 sand.

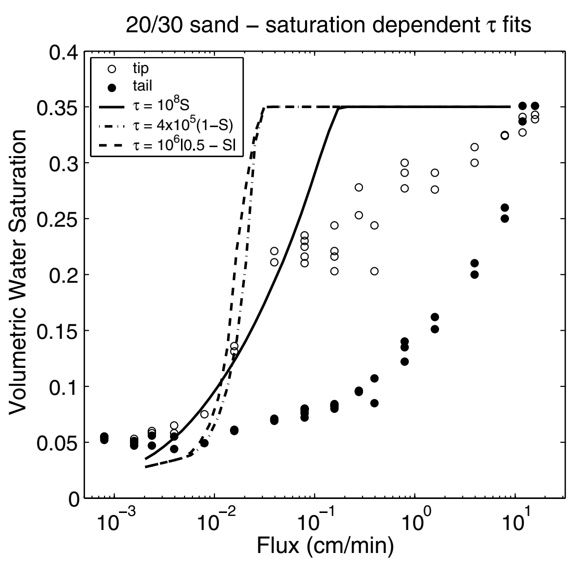

Fig. 5. Best fits using different saturation dependent τ's. An increasing τ with saturation provides the best fit, but with costs mentioned in the text.

vide no benefit. The best fit was found using a τ that increased linearly with saturation (case (a)), where the fit to the tip water content was better than the constant τ case. Unfortunately, this came at a high cost, as the overall profiles (water content versus z, as in Fig. 1) obtained at intermediate fluxes (between 0.01 and 0.1 cm/min) were unphysical in the sense that the predicted distance from dry soil to the tip was on the order of 10 cm, much longer than the sub-centimeter fringe seen in the experiments. Thus it appears that simple saturation dependent τ's do not improve the quality of the fit to the data.

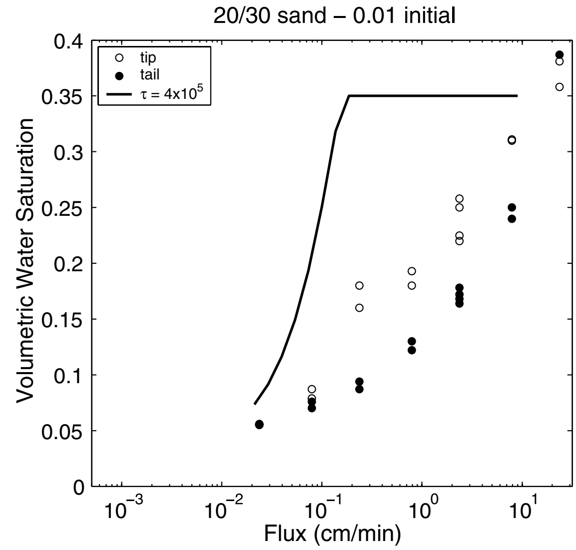

Fig. 6. Calculated overshoot tip saturations (solid line) versus flux for 20/30 sand with an initial water content of 0.01 compared to experimentally measured tip and tail saturations [3]. The value of τ used was obtained from the dry 20/30 sand, and does not provide a good fit to initially wet sand.

In addition, comparisons can also be made between the theory and experiment when the soil is not dry but has an initial water content. Fig. 6 shows the predicted overshoot as a function of flux (using τ from the dry 20/30 sand) and the experimental observations for the 20/30 sand with initial water content of 0.01 [3]. The match is very poor, but this is not strong evidence against the validity of the approach as the soil imbibition curves are likely to be significantly different when there is an initial water content, and these curves are currently unmeasured.

4. Discussion

It is seen that saturation overshoot can be produced using a dynamic nonequilibrium pressure as advocated by Hassanizadeh and Gray [13,12] among others. Using a constant τ term as suggested as a first cut [12] the flux range for which saturation overshoot occurs can be matched well, using values of τ consistent with those found previously [12]. While the overshoot range can be fit to match decently with the data, the constant τ term consistently predicts a large flux region where the tips are saturated fully. This is not seen experimentally for any of the sands measured previously. Using a saturation dependent τ is not seen to improve the match to the experimental data.

More importantly, the magnitude of τ needs to be adjusted orders of magnitude to fit the data for each different sand. In particular, the 12/20 sand grains are only about 50% bigger than the 20/30 sand grains (and similar in shape [20]), but require a τ of a factor of 10 greater to get the flux range correct. Hassanizadeh et al. [12] suggested that τ may vary with grain size. They cite Stauffer [22] who suggested the following empirical dependence of τ on soil properties

$$\tau \propto \frac{\phi\mu}{K\lambda}(p^e)^2, \tag{19}$$

where μ is the viscosity, p^e is the Brooks–Corey entry pressure in units of head (inversely proportional to the α of the van Genuchten parameters (Table 1)), and λ is the Brooks–Corey shape factor (related to n in the van Genuchten parameters). Hassanizadeh et al. [12] point out that this predicts a larger τ for finer grained media, and they find this qualitatively true for imbibition but not drainage. In any case, using the 20/30 and 12/20 soil parameters in Table 1, this predicts a τ smaller by a factor of 5 for the 12/20 than the 20/30, while the fits suggest a τ greater by a factor of 10, exactly the opposite.

For the grey sand, a τ smaller by a factor of 10 is required when compared to the 20/30 sand. This is in the correct direction predicted by Eq. (19), although the sands are not Miller [15] similar (the grey sand has angular grains, and the 20/30 has smooth grains). Most importantly, the 12/20 and the grey sands have very similar imbibition and drainage characteristics (the traditional constitutive relationships [3]), but require nonequilibrium terms a factor of 100 different than each other to model the results. It is not surprising that sands with different physical shapes (all other quantities being equal) would have different nonequilibrium terms, but the magnitude of this difference is huge.

Naturally, one would ideally prefer to add a small term to the continuum Richards equation to model the observed saturation overshoot seen on infiltration. These results question the efficacy of such a method, mainly due to the fact that the needed extra term has parameters which vary greatly from soil to soil, and needs to be fit to the results to be effective. If the magnitude of the nonequilibrium term can be found using some other measurement, and this compared to the infiltration experiments, then the procedure would have more validity and usability.

There are strong conceptual arguments that in cases of saturation overshoot and gravity driven fingering that the front is so sharp at the pore scale that a continuum modeling approach is fraught with difficulties due to the fact that a continuum scale cannot be well defined for fronts sharp at the pore scale [1]. For the solutions presented here, the length scale over which the saturation changes at the front is roughly 2 cm (see Fig. 1), which is well into the continuum region. Thus this continuum model is at least self consistent for these infiltrations, although the match to the experimental observed profile (which have sharp fronts with saturation changes taking place at the sub-centimeter scale) is poor.

In summary, it is straightforward to add additional continuum terms to the Richards equation, and to obtain traveling wave solutions like those observed for constant flux infiltrations. Although many of the experimental observations can be matched (overshoot is observed, nonequilibrium parameters needed are of roughly the correct order of magnitude), others cannot (tip saturations are too high, saturation profiles are not as abrupt as observed), and matches that can be made require large adjustments of the nonequilibrium term for small soil changes. This makes the nonequilibrium addition unlikely to provide any predictive capabilities.

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